

Numerical Clifford Analysis for Nonlinear Schrödinger Problem

P. Cerejeiras*
pceres@mat.ua.pt

N. Faustino*
nfaust@mat.ua.pt

N. Vieira*
nvieira@mat.ua.pt

February 1, 2008

Abstract

The aim of this work is to study the numerical solution of the non-linear Schrödinger problem using a combination between Witt basis and finite difference approximations. We construct a discrete fundamental solution for the non-stationary Schrödinger operator and we show the convergence of the numerical scheme. Numerical examples are given at the end of the paper

Keywords: Nonlinear Schrödinger equation, Parabolic Dirac operators, Finite difference methods

MSC 2000: Primary: 65M06; Secondary: 35A08, 15A66, 65J15.

1 Introduction

In this paper we make use of Clifford analysis tools in order to treat a well-known partial differential equation of mathematical physics. This treatment is based on the work developed by K. Gürlebeck and W. Spröbig in [1] and it is (partially) based on an orthogonal decomposition of the underlying function space in terms of the subspace of null-solutions of the corresponding Dirac operator. While the orthogonal decomposition of Gürlebeck and Spröbig has been applied with success to PDE's such as Lamé equations, Maxwell equations and Navier-Stokes equations [2], it works for the stationary case only.

In [3] an alternative approach was proposed, based on an adding of extra basis elements, namely, of a Witt basis. This approach allows the application

*Departamento de Matemática, Universidade de Aveiro, Portugal

of the already existent techniques of elliptic function theory developed in [1] to time-varying domains. A suitable orthogonal decomposition for the underlying function space is, therefore, obtained in terms of the kernel of the positive parabolic Dirac operator and its range after application to a Sobolev space with zero boundary values.

After some basic notions about Clifford algebras presented in the next section, we will define, in Section 2, a generalization of the parabolic Dirac operator introduced in [3] and a generalization of the Teodorescu and Cauchy-Bitsadze operators presented in [1]. Moreover, using the previous definitions we will obtain a factorization of our equation in terms of basis elements of Witt basis and we obtain the fundamental solution for our generic parabolic Dirac operator.

However, the integral representation formulae obtained via this theoretical method are not suitable for an explicit computation of the solution, due to unacceptable convergence rates of the integrals' numerical approximation (see [1] for more details). Hence, to avoid this drawback it becomes necessary to study the discrete analogues of the operators, namely discrete counterparts for the single- and double-layer potentials. Contrary to difference potentials introduced by Ryabenkij [4], where the difference potentials are constructed by means of discrete Green functions, we will introduce in Section 3 difference potentials based on the discrete fundamental solution. An advantage of this approach is that, contrary to discrete Green functions, we will obtain an explicit expression for our discrete fundamental solution $E_{h,-i\tau}$ which is independent of the choice or shape of the domain. In Section 4 we prove the convergence of the discrete counterparts of the analytic operators introduced in Section 2. This will allow us to establish a convergent numerical scheme for the linear non-stationary Schrödinger equation.

In Section 5 we will adapt the previous algorithm in order to solve numerically the cubic Schrödinger equation and we will present in Section 6 some simple numerical examples to show the consistency and stability of our algorithm for different mesh sizes h and τ .

2 Preliminaries

2.1 Clifford algebras

Consider the n -dimensional vector space \mathbb{R}^n endowed with a standard orthonormal basis $\{e_1, \dots, e_n\}$ and satisfying the multiplication rules $e_i e_j + e_j e_i = -2\delta_{i,j}$.

We define the universal Clifford algebra $\mathcal{C}\ell_{0,n}$ as the 2^n -dimensional associative algebra with basis given by $e_0 = 1$ and $e_A = e_{h_1} \cdots e_{h_k}$, where $A = \{h_1, \dots, h_k\} \subset N = \{1, \dots, n\}$, for $1 \leq h_1 < \dots < h_k \leq n$. Each element $x \in \mathcal{C}\ell_{0,n}$ will be represented by $x = \sum_A x_A e_A$ and each non-zero vector $x = \sum_{j=1}^n x_j e_j \in \mathbb{R}^n$ has a multiplicative inverse given by $\frac{-x}{|x|^2}$. We denote by $\bar{x}^{\mathcal{C}\ell_{0,n}}$ the (Clifford) conjugate of the element $x \in \mathcal{C}\ell_{0,n}$, where

$$\bar{1}^{\mathcal{C}\ell_{0,n}} = 1 \quad \bar{e}_j^{\mathcal{C}\ell_{0,n}} = -e_j \quad \overline{ab}^{\mathcal{C}\ell_{0,n}} = \bar{b}^{\mathcal{C}\ell_{0,n}} \bar{a}^{\mathcal{C}\ell_{0,n}}.$$

We introduce the complexified Clifford algebra $\mathcal{C}\ell_n$ as the tensorial product

$$\mathbb{C} \otimes \mathcal{C}\ell_{0,n} = \{w = \sum_A z_A e_A, \ z_A \in \mathbb{C}, A \subset N\},$$

where the imaginary unit interact with the basis elements as $ie_j = e_j i$, $j = 1, \dots, n$.

The conjugation is defined as $\bar{w} = \sum_A \bar{z}_A \bar{e}_A^{\mathcal{C}\ell_{0,n}}$.

We consider the Dirac operator $D = \sum_{j=1}^n e_j \frac{\partial}{\partial x_j}$ which has the property of factorizing the n -dimensional Laplacian, that is, $D^2 = -\Delta$. A $\mathcal{C}\ell_n$ -valued function on an open domain $\underline{\Omega}$, $u : \underline{\Omega} \subset \mathbb{R}^n \mapsto \mathcal{C}\ell_n$, is said to be *left-monogenic* if it satisfies $Du = 0$ on $\underline{\Omega}$.

Let now $\Omega \subset \mathbb{R}^n \times \mathbb{R}^+$ denote a bounded domain with a sufficiently smooth boundary $\Gamma = \partial\Omega$, while $(0, T)$, with $T > 0$, represents its projection on the time-domain. A function $u : \Omega \mapsto \mathcal{C}\ell_n$ has a representation $u = \sum_A u_A e_A$ with \mathbb{C} -valued components u_A . Properties such as continuity will be understood component-wisely. In the following we will use the short notation $L_p(\Omega)$, $C^k(\Omega)$, etc., instead of $L_p(\Omega, \mathcal{C}\ell_n)$, $C^k(\Omega, \mathcal{C}\ell_n)$. For more details, see [5].

Taking into account [3] we will imbed \mathbb{R}^n into \mathbb{R}^{n+2} . For that purpose we add two new basis elements \mathfrak{f} and \mathfrak{f}^\dagger satisfying

$$\mathfrak{f}^2 = \mathfrak{f}^{\dagger 2} = 0, \quad \mathfrak{f}\mathfrak{f}^\dagger + \mathfrak{f}^\dagger\mathfrak{f} = 1, \quad \mathfrak{f}e_j + e_j\mathfrak{f} = \mathfrak{f}^\dagger e_j + e_j\mathfrak{f}^\dagger = 0, \quad j = 1, \dots, n. \quad (1)$$

The set $\{\mathfrak{f}, \mathfrak{f}^\dagger\}$ is said to be a Witt basis for \mathbb{R}^2 and it will allows us to create a suitable factorization of the Schrödinger operator where only partial derivatives are used.

2.2 Factorization of time-evolution operators

In this section we present a new method for factorizing the Schrödinger equation,

$$(\pm i\partial_t - \Delta)u(x, t) = 0, \quad (x, t) \in \Omega, \quad (2)$$

where $\Omega \subset \mathbb{R}^n \times \mathbb{R}^+$ denotes a bounded domain. For this we will follow the ideas presented in [3], [6] and [7].

Definition 2.1. For a function $u \in C^1(\Omega)$ we define the forward (resp. backward) parabolic Dirac operator

$$D_{x,\pm it}u = (D + \mathfrak{f}\partial_t \pm i\mathfrak{f}^\dagger)u, \quad (3)$$

where D stands for the (spatial) Dirac operator.

These operators factorize the correspondent backward/forward time-evolution operator (2), that is

$$(D_{x,\pm it})^2 u = (\pm i\partial_t - \Delta)u. \quad (4)$$

We consider now the generic Stokes' Theorem.

Theorem 2.2. For each $u, v \in W_p^1(\Omega)$, $1 < p < \infty$ it holds

$$\int_{\partial\Omega} v d\sigma_{x,t} u = \int_{\Omega} [(v D_{x,-it})u + v(D_{x,+it}u)] dx dt,$$

where $d\sigma_{x,t} = (D_x + \mathfrak{f}\partial_t) dx dt$ stands for the contraction of the homogeneous operator associated to $D_{x,-it}$ with the volume element.

For the proof of this theorem we refer to [3].

We shall construct a fundamental solution for the backward parabolic Dirac operator $D_{x,-it}$ in terms of a fundamental solution of the backward Schrödinger operator. We recall that the function

$$e_-(x, t) = i \frac{H(t)}{(4\pi it)^{n/2}} \exp\left(i \frac{|x|^2}{4t}\right) \quad (5)$$

is a fundamental solution for the backward Schrödinger operator since it satisfies

$$(-i\partial_t - \Delta)e_-(x, t) = e_-(x, t)(-i\partial_t - \Delta) = \delta(x, t)$$

in distributional sense. Therefore, we have

Definition 2.3. Given a fundamental solution $e_- = e_-(x, t)$ for the backward Schrödinger operator we have as a fundamental solution $E_- = E_-(x, t)$ for the backward parabolic Dirac operator $D_{x,-it}$ the function

$$\begin{aligned} E_-(x, t) &= e_-(x, t) D_{x,-it} \\ &= \frac{H(t) \exp\left(i \frac{|x|^2}{4t}\right)}{(4\pi it)^{n/2}} \left(-\frac{x}{2t} + \mathfrak{f} \left(\frac{|x|^2}{4t^2} - i \frac{n}{2t} \right) + \mathfrak{f}^\dagger \right). \end{aligned} \quad (6)$$

Using the fundamental solution (6) and the generic Borel-Pompeiu formula we construct the adequate Teodorescu and Cauchy-Bitsadze operators.

Definition 2.4. For a function $u \in L_p(\Omega)$, $1 < p < \infty$, we define the correspondent Teodorescu and Cauchy-Bitsadze operators, respectively, as

$$\begin{aligned} Tu(x_0, t_0) &= \int_{\Omega} E_-(x - x_0, t - t_0) u(x, t) dx dt, \\ Fu(x_0, t_0) &= \int_{\partial\Omega} E_-(x - x_0, t - t_0) d\sigma_{x,t} u(x, t). \end{aligned}$$

We also have the following decomposition (c.f. [7]).

Theorem 2.5. The space $L_p(\Omega)$, $1 < p \leq 2$ allows the direct decomposition

$$L_p(\Omega) = L_p(\Omega) \cap \ker(D_{x,+it}) \oplus D_{x,+it} \left(\overset{\circ}{W}_p^1(\Omega) \right),$$

where $\overset{\circ}{W}_p^1(\Omega)$ denotes the space of all functions in the Sobolev space $W_p^1(\Omega)$ with zero-boundary values.

The previous decomposition of the L_p -space allows us to establish two projections operators.

Definition 2.6. Let $1 < p \leq 2$. We define the projectors

$$P : L_p(\Omega) \rightarrow L_p(\Omega) \cap \ker(D_{x,+it}) \quad (7)$$

and

$$Q : L_p(\Omega) \rightarrow D_{x,+it} \left(\overset{\circ}{W}_p^1(\Omega) \right). \quad (8)$$

Theorem 2.7. Let $f \in L_p(\Omega)$, for $1 < p \leq 2$. The solution of the forward linear Schrödinger problem

$$\begin{cases} i \frac{\partial u}{\partial t} - \Delta u &= f \text{ in } \Omega \\ u &= 0 \text{ on } \partial\Omega \end{cases}$$

is then given by $u = TQTf$.

The proof of this theorem was made in [7] for the case of $p = 2$. However, we remark that it can easily be extended to $1 < p < 2$. Moreover,

1) we can obtain dual results for the backward Schrödinger problem by considering a fundamental solution for the forward parabolic Dirac operator $D_{x,+it}$ on Theorem 2.2;

2) the above construction can easily be generalized for arbitrary operators of type $a\partial_t - \Delta$, where a is a non-zero complex parameter. Indeed, the case of $a = 1$ gives the well-known heat equation while for $a = i$ we have the non-stationary Schrödinger equation.

3 Discrete fundamental solution for the time-evolution problem

3.1 Quaternionic matrix representation of the Witt Basis

We use the matrix representation of the generators of the real quaternions as defined in [1],

$$\mathbf{e}_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{e}_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$\mathbf{e}_2 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \mathbf{e}_3 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

as representatives of a discrete version of the spatial basis for the quaternionic case.

3.2 Finite differences and time evolution operators

As already stated we want to investigate a finite difference scheme based on the notion of a discrete fundamental solution as described in [8]. We denote by

$$\mathbb{R}_h^3 = \{h\underline{m} = (hm_1, hm_2, hm_3), m_l \in \mathbb{Z}\} \quad \text{and} \quad \mathbb{R}_\tau^+ = \{k\tau, k \in \mathbb{Z}^+\}$$

equidistant lattices corresponding to space and time discretization, respectively. For a discrete function $u : \mathbb{R}_h^3 \times \mathbb{R}_\tau^+ \rightarrow \mathbb{C}^4 \sim \mathbb{C} \otimes \mathbb{H}$, $u(h\underline{m}, k\tau) = (u^0, u^1, u^2, u^3)$, we have the finite difference approximation for the stationary Dirac operators given by

$$D_h^{-+}u = \begin{pmatrix} -\partial_h^{-1}u^1 - \partial_h^{-2}u^2 - \partial_h^{-3}u^3 \\ \partial_h^{-1}u^0 - \partial_h^3u^2 + \partial_h^2u^3 \\ \partial_h^{-2}u^0 + \partial_h^3u^1 - \partial_h^1u^3 \\ \partial_h^{-3}u^0 - \partial_h^2u^1 + \partial_h^1u^2 \end{pmatrix}, \quad D_h^{+-}u = \begin{pmatrix} -\partial_h^1u^1 - \partial_h^2u^2 - \partial_h^3u^3 \\ \partial_h^1u^0 - \partial_h^{-3}u^2 + \partial_h^{-2}u^3 \\ \partial_h^2u^0 + \partial_h^{-3}u^1 - \partial_h^{-1}u^3 \\ \partial_h^3u^0 - \partial_h^{-2}u^1 + \partial_h^{-1}u^2 \end{pmatrix},$$

$$uD_h^{-+} = \begin{pmatrix} -\partial_h^{-1}u^1 - \partial_h^{-2}u^2 - \partial_h^{-3}u^3 \\ \partial_h^{-1}u^0 + \partial_h^3u^2 - \partial_h^2u^3 \\ \partial_h^{-2}u^0 - \partial_h^3u^1 + \partial_h^1u^3 \\ \partial_h^{-3}u^0 + \partial_h^2u^1 - \partial_h^1u^2 \end{pmatrix}, \quad uD_h^{+-} = \begin{pmatrix} -\partial_h^1u^1 - \partial_h^2u^2 - \partial_h^3u^3 \\ \partial_h^1u^0 + \partial_h^{-3}u^2 - \partial_h^{-2}u^3 \\ \partial_h^2u^0 - \partial_h^{-3}u^1 + \partial_h^{-1}u^3 \\ \partial_h^3u^0 + \partial_h^{-2}u^1 - \partial_h^{-1}u^2 \end{pmatrix},$$

where

$$\partial_h^{\pm s} u^j = \frac{(u^j(h\underline{m} \pm h e_s, k\tau) - u^j(h\underline{m}, k\tau))}{h}, \quad j = 0, 1, 2, 3, \quad s = 1, 2, 3,$$

represent the spatial forward/backward difference operators. We remark that these difference Dirac operators factorize the star discretization of the Laplace operator, in the sense that

$$D_h^{+-} D_h^{-+} = D_h^{-+} D_h^{+-} = -\Delta_h \mathbf{e}_0 = \left(\sum_{s=1}^3 \partial_h^{-s} \partial_h^s \right) \mathbf{e}_0.$$

Moreover, we also have the following (forward) time difference operator (see [1], [8])

$$\partial_\tau u^j(h\underline{m}, k\tau) = \frac{u^j(h\underline{m}, (k+1)\tau) - u^j(h\underline{m}, k\tau)}{\tau}, \quad j = 0, \dots, 3.$$

With the previous definitions we aim to construct a finite difference approximation for the parabolic Dirac operators. For this purpose we introduce the matrix representations

$$D_{h,\pm i\tau} = \begin{pmatrix} \mathbf{0} & D_h^{+-} \\ D_h^{+-} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix} \gamma^\pm \pm \begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix} \gamma^\mp, \quad (9)$$

where γ^+, γ^- denote elements which satisfy the following matricial operations

$$\begin{aligned} \gamma^\pm \begin{pmatrix} A & B \\ C & D \end{pmatrix} &= \begin{pmatrix} A & -B \\ -C & D \end{pmatrix} \gamma^\pm, \\ (\gamma^\pm)^2 &= 0, \\ \gamma^+ \gamma^- + \gamma^- \gamma^+ &= id. \end{aligned} \quad (10)$$

Using the properties of the previous operators and taking account the

multiplication rules (10) we obtain the following relation

$$\begin{aligned}
(D_{h,\pm i\tau})^2 &= \left[\begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix} \gamma^+ \pm \begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix} \gamma^- \right]^2 \\
&= \left[\begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix} \right]^2 + \left[\begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix} \gamma^+ \right]^2 + \left[\begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix} \gamma^- \right]^2 + \\
&\quad \left[\begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix} \gamma^+ + \begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix} \gamma^+ \begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix} \right] \pm \\
&\quad \left[\begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix} \begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix} \gamma^- + \begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix} \gamma^- \begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix} \right] \pm \\
&\quad \left[\begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix} \gamma^+ \begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix} \gamma^- + \begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix} \gamma^- \begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix} \gamma^+ \right] \\
&= \begin{pmatrix} -\Delta_h & \mathbf{0} \\ \mathbf{0} & -\Delta_h \end{pmatrix} + \left[\begin{pmatrix} \mathbf{0} & \partial_\tau D_h^{-+} \\ \partial_\tau D_h^{+-} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & -\partial_\tau D_h^{-+} \\ -\partial_\tau D_h^{+-} & \mathbf{0} \end{pmatrix} \right] \gamma^\pm \pm \\
&\quad \left[\begin{pmatrix} \mathbf{0} & iD_h^{-+} \\ iD_h^{+-} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & -iD_h^{-+} \\ -iD_h^{+-} & \mathbf{0} \end{pmatrix} \right] \gamma^\mp \pm \begin{pmatrix} i\partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\partial_\tau \mathbf{e}_0 \end{pmatrix} (\gamma^+ \gamma^- + \gamma^- \gamma^+) \\
&= (-\Delta_h \pm i\partial_\tau) \begin{pmatrix} \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \mathbf{e}_0 \end{pmatrix} \quad (11)
\end{aligned}$$

i.e., these operators factorize the difference discretization of our time evolution operator (2). Moreover, due to the fact that the above finite difference operators D_h^{-+} , D_h^{+-} and ∂_τ are approximations of the Dirac operator D and of the time partial derivative operator ∂_t , respectively (see [9]), we have that (9) are a finite difference approximations for the parabolic Dirac operators $D_{x,\pm i\tau}$.

3.3 Discrete fundamental solutions

Based on the ideas presented in [9] we introduce the discrete fundamental solution for the Schrödinger difference operator $-i\partial_\tau - \Delta_h$ as

$$e_{h,-i\tau}(h\underline{m}, k\tau) = iH(k\tau)(1 + i\tau\Delta_h)^{k-1} \delta_h(h\underline{m}), \quad (12)$$

where H denotes the Heaviside function and

$$\delta_h(h\underline{m}) = \begin{cases} \frac{1}{h^3} & \text{if } h\underline{m} = \mathbf{0} \\ 0 & \text{if } h\underline{m} \neq \mathbf{0} \end{cases}, \quad \delta_\tau(k\tau) = \begin{cases} \frac{1}{\tau} & \text{if } k\tau = 0 \\ 0 & \text{if } k\tau \neq 0 \end{cases},$$

are the discrete analogues of the Dirac delta function in \mathbb{R}_h^3 and \mathbb{R}_τ , respectively. Easy calculations show that, indeed, we have

$$(-i\partial_\tau - \Delta_h)e_{h,-i\tau}(h\underline{m}, k\tau) = e_{h,-i\tau}(-i\partial_\tau - \Delta_h)(h\underline{m}, k\tau) = \delta_\tau(k\tau)\delta_h(h\underline{m}). \quad (13)$$

By the factorization property (11), we have for the discrete fundamental solution of the operator $D_{h,-i\tau}$ the function

$$E_{h,-i\tau} = e_{h,-i\tau} D_{h,-i\tau}.$$

Moreover, straightforward calculations give the following matrix representation for the discrete fundamental solution $E_{h,-i\tau}$

$$E_{h,-i\tau}(h\underline{m}, k\tau) = \left[\begin{pmatrix} \mathbf{0} & D_h^{-+} e_{h,-i\tau} \\ D_h^{+-} e_{h,-i\tau} & \mathbf{0} \end{pmatrix} + \partial_\tau e_{h,-i\tau} \begin{pmatrix} \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \mathbf{e}_0 \end{pmatrix} \gamma^+ - i e_{h,-i\tau} \begin{pmatrix} \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \mathbf{e}_0 \end{pmatrix} \gamma^- \right]$$

However, it remains to prove that the discrete fundamental solution $e_{h,-i\tau}$ is indeed an approximation of the fundamental solution (5). This will be done in the next section.

4 Discrete operator calculus

We define the discrete l_p -spaces, $1 \leq p < \infty$, in the usual way

$$g \in l_p(\mathbb{R}_h^3 \times \mathbb{R}_\tau^+)$$

iff

$$\|g\|_{l_p(\mathbb{R}_h^3 \times \mathbb{R}_\tau^+)} = \left(\sum_{(h\underline{m}, \tau k) \in \mathbb{R}_h^3 \times \mathbb{R}_\tau^+} h^3 \tau |g(h\underline{m}, \tau k)|^p \right)^{\frac{1}{p}} < \infty.$$

Henceforward, no distinction will be made between the function $u : \Omega \rightarrow \mathbb{C}^4$ and its restriction $u = u(h\underline{m}, k\tau)$ to the lattice $\Omega_{h,\tau} = \Omega \cap (\mathbb{R}_h^3 \times \mathbb{R}_\tau^+)$, this distinction being clear from the context.

4.1 Behavior of the discrete fundamental solution

We now study the behavior of the discrete fundamental solution (12) when h and τ tend to zero and we prove that it converges in l_1 -sense to the restriction to the grid of the fundamental solution (5).

Theorem 4.1. *Let $\frac{\tau}{h^2} < \frac{1}{6\pi^2}$. Then for any bounded domain $G \subset \mathbb{R}^3$ it holds*

$$\|e_{h,-i\tau} - e_-\|_{l_1(G_h \times [0, +\infty)_\tau)} \rightarrow 0$$

as $h, \tau \rightarrow 0$.

The proof of this theorem is based on [10], Theorem 1, after adaptation to space dimension $n = 3$ and taking in account that our solutions differ from the ones in the case of the heat operator by the relations

$$e_-(\cdot, \cdot) = ie(\cdot, i\cdot) \quad (\text{continuous case})$$

and

$$e_{h,-i\tau}(\cdot, \cdot) = ie_{h,\tau}(\cdot, i\cdot), \quad (\text{discrete case}).$$

Moreover, due to the fact that the constructed discrete fundamental solution $e_{h,-i\tau}$ has a conical support domain we obtain the mesh-size condition $\frac{\tau}{h^2} < \frac{1}{6\pi^2}$.

We remark that Theorem 4.1 implies the l_1^{loc} -convergence of (12) to (5). Also, as an immediate consequence we have

Corollary 4.2. *Under the conditions of Theorem 4.1 it holds*

$$\|E_{h,-i\tau} - E_-\|_{l_1(G_h \times [0, +\infty)_\tau)} \rightarrow 0$$

for any bounded discrete domain $G_h \subset \mathbb{R}^3$, as $h, \tau \rightarrow 0$.

While we can prove the convergence of the discrete solution $E_{h,-i\tau}$ to E_- , the proofs do not yield the order of convergence due to the nature of the continuous fundamental solution of the Schrödinger equation. This will be the subject of future work.

Hence, we can establish the discrete analogues of the Teodorescu operator.

Theorem 4.3. *For all $u \in l_p(\Omega_{h,\tau})$, $1 < p < +\infty$, such that $u : \Omega_{h,\tau} \rightarrow \mathbb{C}^4$ we have the discrete Teodorescu operator $T_{h,-i\tau}$ satisfying to*

$$D_{h,-i\tau} T_{h,-i\tau} u(h\underline{m}, k\tau) = u(h\underline{m}, k\tau), \quad (14)$$

where

$$T_{h,-i\tau} u(h\underline{m}, k\tau) = \sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}} h^3 \tau E_{h,-i\tau}(h\underline{m} - h\underline{n}, k\tau - s\tau) u(h\underline{n}, s\tau), \quad (15)$$

for all $(h\underline{m}, k\tau) \in \Omega_{h,\tau}$.

Proof. We have for $T_{h,-i\tau}$ that

$$D_{h,-i\tau} T_{h,-i\tau} u(h\underline{m}, k\tau) = \sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}} h^3 \tau [D_{h,-i\tau} E_{h,-i\tau}](h\underline{m} - h\underline{n}, k\tau - s\tau) u(h\underline{n}, s\tau).$$

Since $E_{h,-i\tau} = e_{h,-i\tau} D_{h,-i\tau}$ and $e_{h,-i\tau}$ is a scalar solution, we have

$$\begin{aligned}
& D_{h,-i\tau} T_{h,-i\tau} u(h\underline{m}, k\tau) \\
&= \sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}} h^3 \tau [e_{h,-i\tau} (D_{h,-i\tau})^2 (h\underline{m} - h\underline{n}, k\tau - s\tau)] u(h\underline{n}, s\tau) \\
&= \sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}} h^3 \tau [\delta_h(h\underline{m} - h\underline{n}) \delta_\tau(k\tau - s\tau) u(h\underline{n}, s\tau)] \\
&= u(h\underline{m}, k\tau).
\end{aligned}$$

□

Now we are able to present the following norm estimate.

Theorem 4.4. *For all $u \in l_p(\Omega_{h,\tau})$, $1 < p < +\infty$, such that $u : \Omega_{h,\tau} \rightarrow \mathbb{C}^4$ there exists a positive constant $C > 0$ such that*

$$\|T_{h,-i\tau} u\|_{l_p(\Omega_{h,\tau})} \leq C \|u\|_{l_p(\Omega_{h,\tau})}.$$

Moreover, $T_{h,-i\tau}$ is a continuous operator.

Proof. Initially we have

$$\begin{aligned}
& \|T_{h,-i\tau} u\|_{l_p(\Omega_{h,\tau})} = \\
&= \left(\sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}} \tau h^3 |E_{h,-i\tau}(h\underline{m} - h\underline{n}, k\tau - s\tau) u(h\underline{n}, s\tau)|^p \right)^{\frac{1}{p}} \\
&\leq \left(\sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}} \tau h^3 |E_{h,-i\tau}(h\underline{m} - h\underline{n}, k\tau - s\tau)|^p |u(h\underline{n}, s\tau)|^p \right)^{\frac{1}{p}}.
\end{aligned}$$

Let us take $C(\underline{m}, k) = \max_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}} |E_{h,-i\tau}(h\underline{m} - h\underline{n}, k\tau - s\tau)|$. Then there exists $C = \max C(\underline{m}, k) > 0$, this maximum being taken over all (\underline{m}, k) such that $(h\underline{m}, k\tau) \in \Omega_{h,\tau}$, and the result holds. □

As we have done for the analytic case we can establish a decomposition of the l_p -space.

Theorem 4.5. *For the space $l_p(\Omega_{h,\tau})$, $1 < p < \infty$, the following direct decomposition*

$$l_p(\Omega_{h,\tau}) = \ker D_{h,-i\tau}(\text{int}\Omega_{h,\tau}) \oplus D_{h,-i\tau}(w_p^1(\Omega_{h,\tau}))$$

is valid, with correspondent discrete projection operators

$$\begin{aligned} P_{h,\tau} &: l_p(\Omega_{h,\tau}) \mapsto \ker D_{h,-i\tau}(\text{int}\Omega_{h,\tau}), \\ Q_{h,\tau} &: l_p(\Omega_{h,\tau}) \mapsto D_{h,-i\tau}(w_p^1(\Omega_{h,\tau})), \end{aligned}$$

where $w_p^1(\Omega_{h,\tau})$ denotes the discrete counterpart of the Sobolev space $W_p^1(\Omega)$.

4.2 Convergence of the discrete operators

We say that $u \in C^{1,\alpha}(\Omega)$ if its first derivatives are α -Hölder continuous.

Theorem 4.6. *Let $u \in C^{1,\alpha}(\Omega)$. Then it holds $T_{h,-i\tau}u \rightarrow Tu$ as h, τ tend to zero.*

Proof. In order to prove the above result we introduce the regularized Teodorescu operator (see [11])

$$T^\varepsilon u(x, t) = \int_{\Omega} E_-^\varepsilon(x - z, t - r) u(z, r) dz dr,$$

where

$$E_-^\varepsilon(x, t) = e^{-\varepsilon \frac{|x|^2}{4t}} E_-(x, t)$$

stands for a regularization of the fundamental (continuous) solution E_- and, therefore, it converges in the sense of tempered distributions to E_- as $\varepsilon \rightarrow 0$. In a similar way, we construct the regularized discrete operator $T_{h,-i\tau}^\varepsilon$ in terms of the discrete analogue of the regularized fundamental solution

$$E_{h,-i\tau}^\varepsilon = e^{-\varepsilon \frac{|h\underline{m}|^2}{4k\tau}} E_{h,-i\tau}.$$

By definition, we have

$$\begin{aligned} & |T_{h,-i\tau}^\varepsilon u(h\underline{m}, k\tau) - T^\varepsilon u(h\underline{m}, k\tau)| \\ & \leq \left| \sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}} E_{h,-i\tau}^\varepsilon(h\underline{m} - h\underline{n}, k\tau - s\tau) u(h\underline{n}, s\tau) h^3 \tau \right. \\ & \quad \left. - \int_{\Omega} E_-^\varepsilon(h\underline{m} - z, k\tau - r) u(z, r) dz dr \right|. \end{aligned} \quad (16)$$

Due to the singularity of the continuous fundamental solution E_-^ε , we will split the continuous domain Ω into parallelepiped $W(h\underline{n}, s\tau)$ centered at the points $(h\underline{n}, s\tau)$ of the lattice $\Omega_{h,\tau}$ with side-lengths h and τ , respectively. Furthermore, let $p, q \in \mathbb{N}$ be such that $\frac{1}{p} + \frac{1}{q} = 1$. We have then

$$\begin{aligned}
 (16) \leq & \sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}} \left| [E_{h,-i\tau}^\varepsilon(h\underline{m} - h\underline{n}, k\tau - s\tau) - E_-^\varepsilon(h\underline{m} - h\underline{n}, k\tau - s\tau)] u(h\underline{n}, s\tau) h^3 \tau \right| \\
 & + \left| \sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}} [E_-^\varepsilon(h\underline{m} - h\underline{n}, k\tau - s\tau) u(h\underline{n}, s\tau) h^3 \tau \right. \\
 & \left. - \int_{W(h\underline{n}, s\tau)} E_-^\varepsilon(h\underline{m} - z, k\tau - r) u(z, r) dz dr \right|. \quad (17)
 \end{aligned}$$

We use Hölder's inequality on the first term and by a convenient adding up we get

$$\begin{aligned}
 (17) \leq & \|E_{h,-i\tau}^\varepsilon - E_-^\varepsilon\|_{l_p(\Omega_{h,\tau})} \|u\|_{l_q(\Omega_{h,\tau})} \\
 & + \underbrace{\sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}, z \in W(h\underline{n}, s\tau)} [|E_-^\varepsilon(h\underline{m} - h\underline{n}, k\tau - s\tau) u(h\underline{n}, s\tau) - u(z, r)] h^3 \tau|}_{(I_1)} \\
 & + \underbrace{\int_{W(h\underline{n}, s\tau)} |[E_-^\varepsilon(h\underline{m} - h\underline{n}, k\tau - s\tau) - E_-^\varepsilon(h\underline{m} - z, k\tau - r)] u(z, r)| dz dr}_{(I_2(h\underline{n}, s\tau))}.
 \end{aligned}$$

For the term (I_1) we obtain

$$\begin{aligned}
 (I_1) \leq & \sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}, z \in W(h\underline{n}, s\tau)} |E_-^\varepsilon(h\underline{m} - h\underline{n}, k\tau - s\tau)| \\
 & \times \int_{W(h\underline{n}, s\tau)} |u(h\underline{n}, s\tau) - u(z, r)| dz dr \\
 \leq & \sum_{(h\underline{n}, s\tau) \in \Omega_{h,\tau}, z \in W(h\underline{n}, s\tau)} |E_-^\varepsilon(h\underline{m} - h\underline{n}, k\tau - s\tau)| \\
 & \times C \int_{W(h\underline{n}, s\tau)} |(h\underline{n} - z, s\tau - r)|^\alpha dz dr,
 \end{aligned}$$

which goes to zero as $h, \tau \rightarrow 0$.

Finally the term $(I_2(h\underline{n}, s\tau))$ can be estimate using its Taylor series expansion and Hölder's inequality

$$\begin{aligned} (I_2(h\underline{n}, s\tau)) &\leq \int_{W(h\underline{n}, s\tau)} |[E_-^\varepsilon(h\underline{m} - h\underline{n}, k\tau - s\tau) - E_-^\varepsilon(h\underline{m} - z, k\tau - r)] u(z, r)| dz dr \\ &\leq \int_{W(h\underline{n}, s\tau)} |\nabla E_-^\varepsilon(h\underline{m} - z, k\tau - r) \cdot (h\underline{n} - z, s\tau - r)| |u(z, r)| dz dr \\ &\leq \|\nabla E_-^\varepsilon(h\underline{m} - \cdot, k\tau - \cdot) \cdot (h\underline{n} - \cdot, s\tau - \cdot)\|_{L_q(W(h\underline{n}, s\tau))} \|u\|_{L_p(W(h\underline{n}, s\tau))}, \end{aligned}$$

and again we have that $\sum_{(h\underline{n}, s\tau) \in \Omega_{h, \tau}} \sum_{z \in W(h\underline{n}, s\tau)} (I_2(h\underline{n}, s\tau))$ goes to zero as $h, \tau \rightarrow 0$.

Hence, by $\varepsilon \rightarrow 0$ we obtain convergence of the discrete Teodorescu operator $T_{h, -i\tau}$ to the continuous one. \square

Moreover, we notice that we have convergence in $l_p, 1 < p < \infty$, of the regularized discrete Teodorescu operator $T_{h, -i\tau}^\varepsilon$ to the regularized continuous operator T^ε .

We now prove the convergence of the discrete Cauchy-Bitsadze operator $F_{h, -i\tau} = I - T_{h, -i\tau} D_{h, -i\tau}$. Moreover, in what follows we will consider the sub-domains $\Omega^t = \{x \in \mathbb{R}^3 : (x, t) \in \Omega\}$ and $\Omega^x = \{t \in \mathbb{R}^+ : (x, t) \in \Omega\}$.

Theorem 4.7. *If $u \in \ker D_{x, -it}$ is such that $u \in C^{1, \alpha}(\Omega)$ for some $0 < \alpha < 1$ then we have*

$$\|u - F_{h, -i\tau} u\|_{l_p(\Omega_{h, \tau})} \leq C \|u\|_{C^{1, \alpha}(\Omega)} (h^\alpha + \tau^\alpha),$$

for a positive constant $C > 0$.

Proof. We use the definition of $F_{h, -i\tau}$, Theorem 4.4 and the fact that $u \in \ker D_{x, -it}$. We get then

$$\begin{aligned} \|u - F_{h, -i\tau} u\|_{l_p(\Omega_{h, \tau})} &= \|T_{h, -i\tau} D_{h, -i\tau} u\|_{l_p(\Omega_{h, \tau})} \\ &= \|T_{h, -i\tau} (D_{h, -i\tau} u - D_{x, -it} u)\|_{l_p(\Omega_{h, \tau})} \\ &\leq C_1 \|D_{h, -i\tau} u - D_{x, -it} u\|_{l_p(\Omega_{h, \tau})} \\ &\leq C_1 \left(\|D_h u - D_x u\|_{l_p(\Omega_{h, \tau})} + \|\partial_\tau u - \partial_t u\|_{l_p(\Omega_{h, \tau})} \right) \\ &\leq C_1 \left[\left(\sum_{(h\underline{m}, k\tau) \in \Omega_{h, \tau}} |D_h u(h\underline{m}, k\tau) - D_x u(h\underline{m}, k\tau)|^p h^3 \tau \right)^{\frac{1}{p}} \right. \\ &\quad \left. + \left(\sum_{(h\underline{m}, k\tau) \in \Omega_{h, \tau}} |\partial_\tau u(h\underline{m}, k\tau) - \partial_t u(h\underline{m}, k\tau)|^p h^3 \tau \right)^{\frac{1}{p}} \right] \quad (18) \end{aligned}$$

Additionally, we remark that $u \in C^{1,\alpha}(\Omega)$ implies both

$$u(\cdot, t) \in C^{1,\alpha}(\Omega^t), \quad u(x, \cdot) \in C^{1,\alpha}(\Omega^x).$$

Moreover, we have (c.f. [1], p.268) that

$$|D_h^{+-}u(h\underline{m}, k\tau) - D_x u(h\underline{m}, k\tau)| \leq K(k\tau) \|u(\cdot, k\tau)\|_{C^{1,\alpha}(\Omega^{k\tau})} h^\alpha, \quad (19)$$

a similar result holding for D_h^{-+} , and

$$|\partial_\tau(h\underline{m}, k\tau) - \partial_t u(h\underline{m}, k\tau)| \leq K(h\underline{m}) \|u(h\underline{m}, \cdot)\|_{C^{1,\alpha}(\Omega^{h\underline{m}})} \tau^\alpha, \quad (20)$$

for some positive constants $K(k\tau), K(h\underline{m})$. Using these two inequalities we have

$$\begin{aligned} (18) \leq C_1 & \left[\left(\sum_{(h\underline{m}, k\tau) \in \Omega_{h,\tau}} K^p(k\tau) \|u(\cdot, k\tau)\|_{C^{1,\alpha}(\Omega^{k\tau})}^p h^{p\alpha} h^3 \tau \right)^{1/p} \right. \\ & \left. + \left(\sum_{(h\underline{m}, k\tau) \in \Omega_{h,\tau}} K^p(h\underline{m}) \|u(h\underline{m}, \cdot)\|_{C^{1,\alpha}(\Omega^{h\underline{m}})}^p \tau^{p\alpha} h^3 \tau \right)^{1/p} \right]. \end{aligned}$$

We now take $K = \max_{\Omega_{h,\tau}} \{K(k\tau), K(h\underline{m})\} > 0$ and we recall that

$$\|u(h\underline{m}, \cdot)\|_{C^{1,\alpha}(\Omega^{h\underline{m}})} \leq \|u\|_{C^{1,\alpha}(\Omega)}, \quad \|u(\cdot, k\tau)\|_{C^{1,\alpha}(\Omega^{k\tau})} \leq \|u\|_{C^{1,\alpha}(\Omega)}.$$

Hence

$$(18) \leq C_1 K Vol(\Omega_{h,\tau}) \|u\|_{C^{1,\alpha}(\Omega)} (h^\alpha + \tau^\alpha).$$

□

We are now in conditions to prove the convergence of the discrete projection operator $Q_{h,\tau}$ to its continuous counterpart (8).

Theorem 4.8. *Let $u \in L_p(\Omega)$ for some $1 < p < \infty$. Then it holds for the projector $Q_{h,\tau}$*

$$\|Q_{h,\tau}u - Qu\|_{l_p(\Omega_{h,\tau})} \rightarrow 0 \quad \text{as } h, \tau \rightarrow 0$$

for a positive constant C .

Proof. We start from the equality

$$\begin{aligned} Q_{h,\tau}u - Qu &= Q_{h,\tau}(Pu + Qu) - Q(Pu + Qu) \\ &= Q_{h,\tau}Pu + Q_{h,\tau}Qu - Qu \end{aligned}$$

and we wish to obtain estimates for the terms $Q_{h,\tau}Pu$ and $(Q_{h,\tau} - I)Qu$ (we recall that, being projection operators, $Q(Pu) = 0$ and $Q^2 = Q$).

Since $Pu = FPu$ and $Q_{h,\tau}F_{h,-i\tau}u = 0$, for the first term we obtain

$$\begin{aligned} Q_{h,\tau}Pu &= Q_{h,\tau}FPu - Q_{h,\tau}F_{h,-i\tau}Pu \\ &= Q_{h,\tau}(F - F_{h,-i\tau})Pu \\ &= Q_{h,\tau}(I - F_{h,-i\tau} - TD_{x,-it})Pu \\ &= Q_{h,\tau}(I - F_{h,-i\tau})Pu \end{aligned}$$

and, therefore, by Theorem 4.7 we get the following estimate

$$\begin{aligned} \|Q_{h,\tau}Pu\|_{l_p(\Omega_{h,\tau})} &\leq \|Q_{h,\tau}\| \|Pu - F_{h,-i\tau}Pu\|_{l_p(\Omega_{h,\tau})} \\ &\leq C\|Q_{h,\tau}\| \|Pu\|_{C^{1,\alpha}(\Omega)}(h^\alpha + \tau^\alpha), \end{aligned}$$

taking in account that $Q_{h,\tau}$ has bounded norm. Moreover, due to the fact that P is the projection into the kernel of $D_{h,-i\tau}$, it holds $\|Pu\|_{C^{1,\alpha}(\Omega)} < \infty$.

For the second term we remember that Qu can be written as $Qu = D_{x,-it}g$ where $g \in \overset{\circ}{W}_2^1(\Omega)$. This leads to

$$\begin{aligned} (Q_{h,\tau} - I)Qu &= (Q_{h,\tau} - I)D_{x,-it}g \\ &= Q_{h,\tau}(D_{x,-it}g - D_{h,-i\tau}g) + Q_{h,\tau}D_{h,-i\tau}g - D_{x,-it}g \\ &= Q_{h,\tau}(D_{x,-it}g - D_{h,-i\tau}g) + (D_{h,-i\tau}g - D_{x,-it}g), \end{aligned}$$

since $Q_{h,\tau}D_{h,-i\tau}g = D_{h,-i\tau}g$. Hence, taking into account the previous calculations, Theorem 4.7 and relations (19) and (20) we finally obtain

$$\|(Q_{h,\tau} - I)Qu\|_{l_p(\Omega_{h,\tau})} \leq (\|Q_{h,\tau}\| + 1)\|D_{h,-i\tau}g - D_{x,-it}g\|_{l_p(\Omega_{h,\tau})} \rightarrow 0$$

as h, τ goes to zero. \square

The above discrete operators allow us to establish a discrete equivalent of Theorem 2.7.

Theorem 4.9. *Let $f \in l_2(\Omega_{h,\tau})$. The solution of the discrete Schrödinger problem*

$$\begin{cases} (i\partial_\tau - \Delta_h)u &= f \text{ in } \Omega_{h,\tau} \\ u &= 0 \text{ on } \partial\Omega_{h,\tau} \end{cases}$$

is given by $u = T_{h,-i\tau}Q_{h,\tau}T_{h,-i\tau}f$.

5 The non-linear Schrödinger problem

Let us now consider the non-linear Schrödinger problem

$$\begin{cases} i\partial_t u - \Delta u &= M(u) & \text{in } \Omega \\ u &= 0 & \text{on } \partial\Omega \end{cases}$$

where $M(u) = |u|^2 u + f$, with $f \in L_2(\Omega)$, and $|u|^2 = \sum_{j=0}^3 (u^j)^2$. This problem can be reduced to

$$u = TQTM(u) \text{ in } \Omega, \quad (21)$$

a problem for which the next theorem proves existence and uniqueness of solution (see [6], [7] for details).

Theorem 5.1. *The problem (21) has an unique solution given in terms of the iterative method*

$$u_{n+1} = TQTM(u_n)$$

if $f \in L_2(\Omega)$ satisfies the condition

$$\|f\|_{L_2} \leq \frac{1}{36 \cdot 2^{m+1}}.$$

Moreover, the iteration method converges for each starting point $u_0 \in \overset{\circ}{W}_2^1(\Omega)$ such that

$$\|u_0\|_{L_2} \leq \frac{1}{6 \cdot 2^{m+1}} + W,$$

with $W = \sqrt{\frac{1}{36 \cdot 2^{2(m+1)}} - \frac{\|f\|_{L_2}}{2^{m+1}}}$.

Based on the discrete operators previously introduced we construct the discrete version of problem (21) for our bounded domain

$$u = T_{h,-i\tau} Q_{h,\tau} T_{h,-i\tau} M(u) \text{ in } \Omega_{h,\tau}. \quad (22)$$

Indeed, let v be a solution of (22). Then

$$\begin{aligned} (i\partial_\tau - \Delta_h)v &= D_{h,-i\tau} D_{h,-i\tau} [T_{h,-i\tau} Q_{h,\tau} T_{h,-i\tau} M(v)] \\ &= D_{h,-i\tau} [Q_{h,\tau} T_{h,-i\tau} M(v)] \\ &= M(v), \end{aligned}$$

and due to the properties of the projector $Q_{h,\tau}$ we have $v = 0$ on $\partial\Omega_{h,\tau}$.

Using the same ideas as in the continuous case (see [7]) we get results regarding the convergence and uniqueness of the discrete iterative method $u_{n+1} = T_{h,-i\tau} Q_{h,\tau} T_{h,-i\tau} M(u_n)$.

Theorem 5.2. *If $f \in l_2(\Omega_{h,\tau})$ then the discrete problem (22) has a unique solution $u \in \overset{\circ}{w}_2^1(\Omega_{h,\tau})$ whenever*

$$\|f\|_{l_2(\Omega_{h,\tau})} \leq \frac{1}{36C_{h,\tau}}$$

and the initial term $u_0 \in \overset{\circ}{w}_2^1(\Omega_{h,\tau})$ satisfies

$$\|u_0\|_{l_2(\Omega_{h,\tau})} \leq \frac{1}{6C_{h,\tau}} + W_{h,\tau},$$

$$\text{with } W_{h,\tau} = \sqrt{\frac{1}{36C_{h,\tau}} - \frac{\|f\|_{l_2(\Omega_{h,\tau})}}{C_{h,\tau}}}.$$

The proof of this theorem, being similar to the one in the continuous case, will be omitted.

The following result shows that the solution obtained for the discrete problem, which we will denote by u_* , converges to the solution obtained for the continuous, which we will denote by u . In the proof of the following theorem the restriction of $M(u)$ to the space-time grid will be denote by $M_{h,\tau}(u)$.

Theorem 5.3. *Let $f \in L_2(\Omega)$. Then u_* converges to u in $\Omega_{h,\tau}$ whenever $h, \tau \rightarrow 0$.*

Proof. Again, we need to use the regularized Teodorescu operator. We shall denote $u_*^\epsilon = T_{h,-i\tau}^\epsilon Q_{h,\tau} T_{h,-i\tau}^\epsilon M_{h,\tau}(u_*^\epsilon)$ and $u^\epsilon = T^\epsilon Q T^\epsilon M(u^\epsilon)$. We have

$$\begin{aligned} \|u_*^\epsilon - u^\epsilon\|_{l_2(\Omega_{h,\tau})} &\leq \underbrace{\|T_{h,-i\tau}^\epsilon Q_{h,\tau} T_{h,-i\tau}^\epsilon M_{h,\tau}(u^\epsilon) - T^\epsilon Q T^\epsilon M(u^\epsilon)\|_{l_2(\Omega_{h,\tau})}}_{(\mathbf{I})} \\ &\quad + \|T_{h,-i\tau}^\epsilon Q_{h,\tau} T_{h,-i\tau}^\epsilon (M_{h,\tau}(u_*^\epsilon) - M_{h,\tau}(u^\epsilon))\|_{l_2(\Omega_{h,\tau})} \\ &\leq (\mathbf{I}) + C_{h,\tau} \|u_*^\epsilon - u^\epsilon\|_{l_2(\Omega_{h,\tau})} \left(\|u_*^\epsilon\|_{l_2(\Omega_{h,\tau})} + \|u^\epsilon\|_{l_2(\Omega_{h,\tau})} \right) \end{aligned}$$

which implies that

$$\|u_*^\epsilon - u^\epsilon\|_{l_2(\Omega_{h,\tau})} \leq (\mathbf{I}) \left[1 - C_{h,\tau} \left(\|u_*^\epsilon\|_{l_2(\Omega_{h,\tau})} + \|u^\epsilon\|_{l_2(\Omega_{h,\tau})} \right) \right]^{-1},$$

where $C_{h,\tau}$ is a positive constant which depends from h and τ . By Theorem 5.2 we can guarantee that

$$\|u_*^\epsilon\|_{l_2(\Omega_{h,\tau})} \leq \frac{1}{6C_{h,\tau}} + W_{h,\tau},$$

with $W_{h,\tau} = \sqrt{\frac{1}{36C_{h,\tau}} - \frac{\|f\|_{l_2(\Omega_{h,\tau})}}{C_{h,\tau}}}$.

This inequality, together with Theorem 5.1, ensures that for sufficiently small h and τ , the following relation

$$1 - C_{h,\tau} \left(\|u_*^\epsilon\|_{l_2(\Omega_{h,\tau})} + \|u^\epsilon\|_{l_2(\Omega_{h,\tau})} \right) > 0$$

holds. Therefore, the convergence of u_* to u depends only on the term **(I)**. Hereby, we have

$$\begin{aligned} \textbf{(I)} &= \|T_{h,-i\tau}^\epsilon Q_{h,\tau} T_{h,-i\tau}^\epsilon M_{h,\tau}(u^\epsilon) - QT^\epsilon M(u^\epsilon)\|_{l_2(\Omega_{h,\tau})} \\ &\leq \underbrace{\|T_{h,-i\tau}^\epsilon Q_{h,\tau} T_{h,-i\tau}^\epsilon (M_{h,\tau}^*(u^\epsilon) - M^*(u^\epsilon))\|_{l_2(\Omega_{h,\tau})}}_{\textbf{(A)}} \\ &+ \underbrace{\|T_{h,-i\tau}^\epsilon Q_{h,\tau} (T_{h,-i\tau}^\epsilon - T^\epsilon) M^*(u^\epsilon)\|_{l_2(\Omega_{h,\tau})}}_{\textbf{(B)}} + \underbrace{\|T_{h,-i\tau}^\epsilon (Q_{h,\tau} - Q) T^\epsilon M^*(u^\epsilon)\|_{l_2(\Omega_{h,\tau})}}_{\textbf{(C)}} \\ &+ \underbrace{\|T_{h,-i\tau}^\epsilon Q_{h,\tau} (T_{h,-i\tau}^\epsilon - T^\epsilon) f\|_{l_2(\Omega_{h,\tau})}}_{\textbf{(D)}} + \underbrace{\|T_{h,-i\tau}^\epsilon (Q_{h,\tau} - Q) T^\epsilon f\|_{l_2(\Omega_{h,\tau})}}_{\textbf{(E)}}, \end{aligned}$$

where $M^*(u^\epsilon) = |u^\epsilon|^2 u^\epsilon$ and $M_{h,\tau}^*(u^\epsilon)$ denotes its restriction to the space-time grid. By Theorem 4.6 we can say that **(B)** and **(D)** tend to zero as $h, \tau \rightarrow 0$. Also, Theorem 4.8 implies the same result for both **(C)** and **(E)**. Finally, for **(A)** we have, from the boundedness of the discrete operators, the following relation

$$\begin{aligned} &\|T_{h,-i\tau}^\epsilon Q_{h,\tau} T_{h,-i\tau}^\epsilon (M_{h,\tau}^*(u^\epsilon) - M^*(u^\epsilon))\|_{l_2(\Omega_{h,\tau})} \\ &\leq \|T_{h,-i\tau}^\epsilon Q_{h,\tau} T_{h,-i\tau}^\epsilon\|_{l_2(\Omega_{h,\tau})} \|M_{h,\tau}^*(u^\epsilon) - M^*(u^\epsilon)\|_{l_2(\Omega_{h,\tau})} \\ &\leq C_1 C_{h,\tau}, \end{aligned}$$

where C_1 is a finite constant and $C_{h,\tau}$ is a constant which depends on h and τ and goes to zero with h and τ . Therefore, **(I)** tends to zero when $h, \tau \rightarrow 0$, thus, proving our result as $\epsilon \rightarrow 0$. \square

6 Numerical Examples

In order to study the rate of convergence of our method for different mesh sizes, we shall present some numerical examples. For simplicity sake, we shall use a cubic space domain $[-a, a]^3$ with an equidistant discretization grid of $(N+1)^3$ points. Also, for the discretization of the time domain we

shall consider an equidistant grid with $M+1$ mesh-points. At this point, we emphasize that the choice of M and N takes into account the restriction $\frac{\tau}{h^2} < \frac{1}{6\pi^2}$ imposed by Theorem 4.1.

For all the examples below we will be presenting a table with the l^1 -error between the approximated solution and the exact solution at given instants of time.

Example 1: As a first example, we consider an exact real-valued C^∞ solution $u = (0, u_1, u_2, u_3)$ for the problem (21), where

$$u_1(x, t) = e^{-x_1} \cos\left(\pi t + \frac{\pi}{2}\right) \sin(\pi x_1 x_2 x_3)$$

$$u_2(x, t) = u_3(x, t) = 0,$$

and the corresponding right hand side $f = i\partial_t u - \Delta u - |u|^2 u$.

In the following table we show the approximation error between the exact solution u and its discrete approximation $u_{h,\tau}$ on the domain $\Omega = [-5, 5]^3 \times [0, 2]$ for different mesh sizes.

Table 1

N	M	t=0	t=0.4	t=0.8
20	450	2.3313×10^{-3}	1.2799×10^{-3}	5.7386×10^{-4}
25	703	1.5265×10^{-3}	8.3774×10^{-4}	3.7642×10^{-4}
30	1013	1.0765×10^{-3}	5.9073×10^{-4}	2.6569×10^{-4}
35	1378	7.9982×10^{-4}	4.3844×10^{-4}	1.9706×10^{-4}
40	1800	6.1732×10^{-4}	3.3895×10^{-4}	1.5228×10^{-4}
45	2278	4.9075×10^{-4}	2.6919×10^{-4}	1.2107×10^{-4}
50	2813	3.9937×10^{-4}	2.1923×10^{-4}	9.8534×10^{-5}
55	3404	3.3132×10^{-4}	1.8193×10^{-4}	8.1714×10^{-5}
N	M	t=1.2	t=1.6	t=2
20	450	2.5728×10^{-4}	1.1633×10^{-4}	5.3040×10^{-5}
25	703	1.6914×10^{-4}	7.5998×10^{-5}	3.4520×10^{-5}
30	1013	1.1950×10^{-4}	5.3548×10^{-5}	2.4266×10^{-5}
35	1378	8.8572×10^{-5}	3.9810×10^{-5}	1.7992×10^{-5}
40	1800	6.8416×10^{-5}	3.0738×10^{-5}	1.3868×10^{-5}
45	2278	5.4362×10^{-5}	2.4450×10^{-5}	1.1014×10^{-5}
50	2813	4.4226×10^{-5}	1.9878×10^{-5}	8.9580×10^{-6}
55	3404	3.6700×10^{-5}	1.6502×10^{-5}	7.4280×10^{-6}

l_1 -error between the approximated solution and the exact solution
at different instants

The following graphics (Figures 1. and 2.) show the evolution of the l_1 -norm for the approximation error, with respect to the space-mesh and to the time-mesh, respectively.

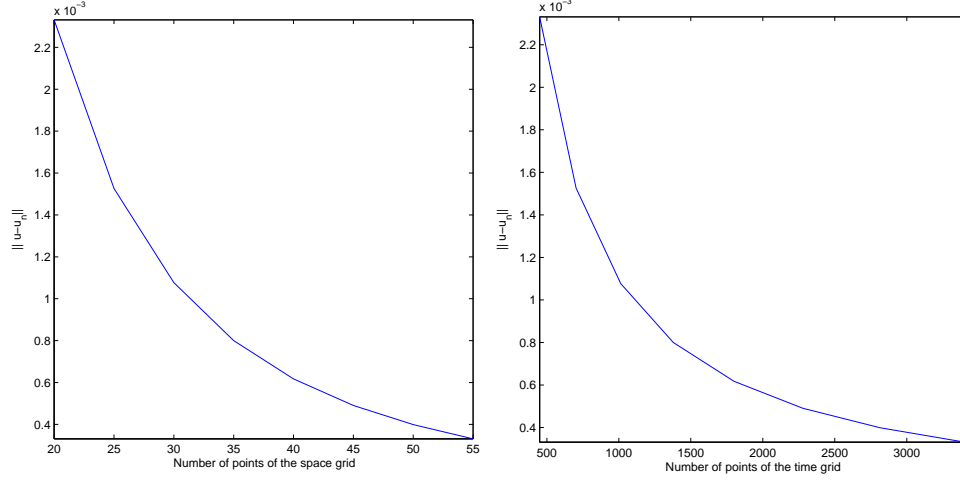


Figure 1: l_1 -error for different space steps. Figure 2: l_1 -error for different time steps.

Example 2: In this example we consider an exact complex-valued C^∞ solution $u = (0, u_1, u_2, u_3)$ of (21), where

$$\begin{aligned} u_1(x, t) &= (e^{-t} - 1) (x_1^2 - 25) (x_2^2 - 25) (x_3^2 - 25) \\ u_2(x, t) &= 0, \quad u_3(x, t) = (e^{-t} - 1) \sin(\pi x_1 x_2 x_3) e^{ix_1 t}. \end{aligned}$$

Below is the table with the error of approximation between the exact solution u and its discrete approximation $u_{h,\tau}$ on the domain $\Omega = [-5, 5]^3 \times [0, 2]$, for different mesh sizes,

Table 2

N	M	t=0	t=0.4	t=0.8
20	450	4.8846×10^{-3}	2.6819×10^{-3}	1.2024×10^{-3}
25	703	3.1692×10^{-3}	1.7323×10^{-3}	7.8152×10^{-4}
30	1013	2.2183×10^{-3}	1.2172×10^{-3}	5.4746×10^{-4}
35	1378	1.6404×10^{-3}	8.9923×10^{-4}	4.4166×10^{-4}
40	1800	1.2613×10^{-3}	6.9250×10^{-4}	3.1112×10^{-4}
45	2278	9.9988×10^{-4}	5.4847×10^{-4}	2.4668×10^{-4}
50	2813	8.1181×10^{-4}	4.4563×10^{-4}	2.0029×10^{-4}
55	3404	6.7227×10^{-4}	3.6914×10^{-4}	1.6580×10^{-4}
N	M	t=1.2	t=1.6	t=2
20	450	5.3907×10^{-4}	2.4374×10^{-4}	1.1140×10^{-5}
25	703	3.5116×10^{-4}	1.5779×10^{-4}	7.1668×10^{-5}
30	1013	2.4623×10^{-4}	1.1033×10^{-4}	5.0000×10^{-5}
35	1378	9.0828×10^{-4}	8.1648×10^{-5}	3.6900×10^{-5}
40	1800	1.8166×10^{-4}	6.2800×10^{-5}	2.8334×10^{-5}
45	2278	1.1076×10^{-4}	4.9816×10^{-5}	2.4428×10^{-5}
50	2813	8.9900×10^{-5}	4.0406×10^{-5}	1.8210×10^{-5}
55	3404	7.4468×10^{-5}	3.3484×10^{-5}	1.5072×10^{-5}

l_1 -error between the approximated solution and the exact solution
at different instants

followed by the graphics (Figures 3. and 4.) of the evolution of the approximation error for the correspondent space and time mesh sizes considered.

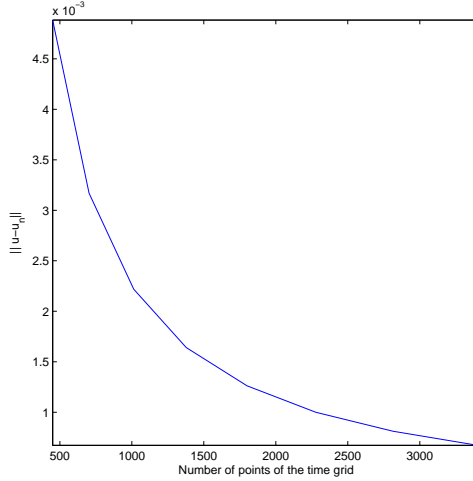
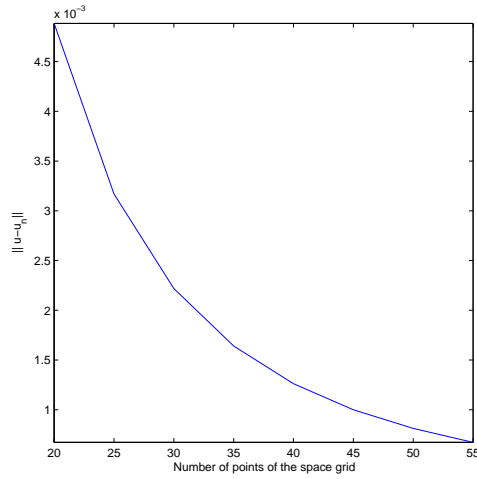


Figure 3: l_1 -error for different space mesh sizes. Figure 4: l_1 -error for different time steps.

Example 3: Finally, we conclude with an example of an exact solution of lower regularity on the domain $\Omega = [-5, 5]^3 \times [0, 2]$, namely an exact C^1 -solution $u = (0, u_1, u_2, u_3)$ of (21), with

$$\begin{aligned} u_1(x, t) &= (e^{-t} - 1) (g(x_1) - g(-x_1)) (g(x_2) - g(-x_2)) (g(x_3) - g(-x_3)) \\ u_2(x, t) &= u_3(x, t) = 0, \end{aligned}$$

where g is the auxiliary B-spline of order 3

$$g(y) = \begin{cases} \frac{y^3}{6} & \text{if } 0 \leq y < 1 \\ -\frac{1}{3} + \frac{y}{2} + \frac{(y-1)^2}{2} - \frac{11(y-1)^3}{24} & \text{if } 1 \leq y < 2 \\ \frac{11}{24} + \frac{y}{8} - \frac{7(y-2)^2}{8} + \frac{3(y-2)^3}{8} & \text{if } 2 \leq y < 3 \\ \frac{11}{6} - \frac{y}{2} + \frac{(y-3)^2}{4} - \frac{(y-3)^3}{24} & \text{if } 3 \leq y \leq 5 \end{cases}.$$

Again, the corresponding right hand side $f = i\partial_t u - \Delta u - |u^2|u$. The following table gives the error of approximation between the exact solution u and its discrete approximation $u_{h,\tau}$ for different mesh sizes considered.

Table 3

N	M	t=0	t=0.4	t=0.8
20	450	5.0846×10^{-3}	2.8819×10^{-3}	1.4024×10^{-3}
25	703	3.7149×10^{-3}	2.0388×10^{-3}	9.1607×10^{-4}
30	1013	2.7242×10^{-3}	1.4948×10^{-3}	6.7232×10^{-4}
35	1378	1.9355×10^{-3}	1.0610×10^{-3}	4.7688×10^{-4}
40	1800	1.4763×10^{-3}	8.1058×10^{-4}	3.6402×10^{-4}
45	2278	1.1856×10^{-3}	6.5030×10^{-4}	2.9248×10^{-4}
50	2813	9.1813×10^{-4}	4.5629×10^{-4}	2.0291×10^{-4}
55	3404	8.0086×10^{-4}	4.3975×10^{-4}	1.9751×10^{-4}
N	M	t=1.2	t=1.6	t=2
20	450	7.3907×10^{-4}	2.4437×10^{-4}	1.9111×10^{-4}
25	703	4.1162×10^{-4}	1.8495×10^{-4}	8.4088×10^{-5}
30	1013	3.0239×10^{-4}	1.3550×10^{-4}	6.1402×10^{-5}
35	1378	2.1434×10^{-4}	9.6336×10^{-5}	4.3534×10^{-5}
40	1800	1.6362×10^{-4}	7.3510×10^{-5}	3.3166×10^{-5}
45	2278	1.3133×10^{-4}	5.9066×10^{-5}	2.6610×10^{-5}
50	2813	9.9006×10^{-5}	4.4078×10^{-5}	1.9410×10^{-5}
55	3404	8.8712×10^{-5}	3.9888×10^{-5}	1.7956×10^{-5}

l_1 -error between the approximated solution and the exact solution
at different instants

The next graphics (Figures 5. and 6.) show the evolution of the approximation error in l_1 -norm for the different space mesh size and time mesh size considered.

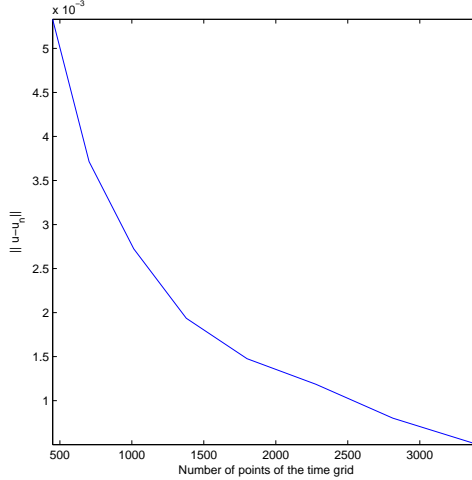
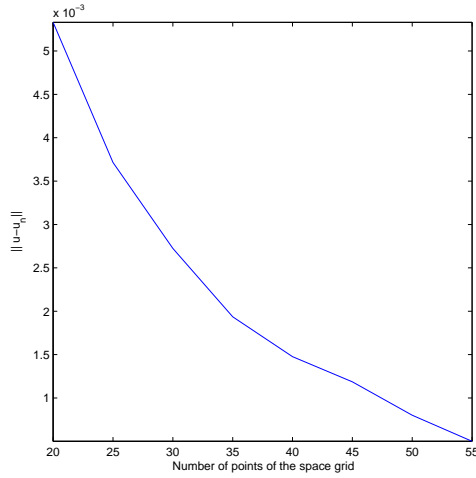


Figure 5: l_1 -error for different space mesh sizes. Figure 6: l_1 -error for different time steps.

Taking into account the previous graphics we are able to observe that the order of convergence for the space coordinate is, in all the examples, of order $\mathcal{O}(h^8)$, while for the time coordinate we get, in all the examples, an order of convergence of order $\mathcal{O}(\tau^{\frac{3}{2}})$. We remark that our method seems to be stable under functions of lower regularity, since the order of convergence for the space and time coordinates remains same in all the three examples.

Acknowledgement The research of the first author was (partially) supported by *Unidade de Investigação “Matemática e Aplicações”* of the University of Aveiro. The work of the second and third authors was supported by PhD-grants SFRH/BD/17657/2004, SFRH/BD/22646/2005, of *Fundação para a Ciência e a Tecnologia*.

References

- [1] K. Gürlebeck and W. Sprößig, “Quaternionic and Clifford calculus for Engineers and Physicists”, John Wiley & Sons, Chichester, 1997.

- [2] V. G. Kravchenko and V. V., Kravchenko, “Quaternionic factorization of the Schrödinger operator and its applications to some first-order systems of mathematical physics”, *J. Phys. A: Math. Gen.* 36, 44 (2000), pp. 11285 – 11297.
- [3] P. Cerejeiras, U. Kähler and F. Sommen, “Parabolic Dirac operators and the Navier-Stokes equations over time-varying domains”, *Math. Meth. in Appl. Sc.* 28, 14(2005), pp. 1715 – 1724.
- [4] V.S. Ryabenkij, “The Method of difference potentials for some for some problems of continuum mechanics”, Nauka, Moskva, 1987 (russian).
- [5] R. Delanghe, F. Sommen and V. Souček, “Clifford algebras and spinor-valued functions”, Kluwer Academic Publishers, Dordrecht, 1992.
- [6] S. Bernstein, “Factorization of the nonlinear Schrödinger equation and applications”, *Compp. Var. and Ellipp. Eq.* - special issue: a tribute to R. Delanghe, 51, n.o 5-6 (2006), pp. 429–452.
- [7] P. Cerejeiras and N. Vieira, “Factorization of the non-linear Schrödinger Operator”, accepted for publication in *Advances in Applied Clifford Algebras*. Available in http://arxiv.org/PS_cache/arxiv/pdf/0704/0704.2304v1.pdf
- [8] K. Gürlebeck and A. Hommel, “On finite difference Dirac operators and their fundamental solutions”, *Adv. Appl. Clifford Algebras* 11, 2001, pp. 89 – 106.
- [9] A. Hommel, “Fundamentallösungen partieller Differentialoperatoren und die Lösung diskreter Randwertprobleme mit Hilfe von Differenzenpotentialen”, Bauhaus-Universität Weimar (Germany), 1998.
- [10] K. Gürlebeck and A. Hommel, “On fundamental solutions of the heat conduction difference operator”, *ZAA* 11, 3 (1994), pp. 1 – 16.
- [11] T. Tao, “Local and global analysis of non-linear dispersive and wave equations”, *CBMS Regional Conference Series in Mathematics*, AMS, 2006.
- [12] H. Holden, K. H. Karlsen and K. A. Lie, “Operator splitting methods for degenerate convection-diffusion equations II: numerical examples with emphasis on reservoir simulation and sedimentation”, *Computational Geosciences* 4 (2000), pp. 287 – 322.